
PUG SOAP Web Service Reference

Table of Contents

PUG SOAP Web Service Reference..... 1

 PUG SOAP Web Service..... 2

 Methods..... 3

 Complex Types..... 36

 Simple Types..... 52

Overview

Description

This document contains Web Service descriptions for the following services.

Web Services

Name	Description
PUG SOAP	

PUG SOAP Web Service

See Also

[Methods](#) | [Complex Types](#) | [Simple Types](#)

Methods: PUG SOAP

Methods

Name	Description
AssayDownload	Given an assay key, prepare for download a file containing an assay data table in the selected format. See the assay query section of the PUG service documentation (http://pubchem.ncbi.nlm.nih.gov/pug/pughelp.html) for more detail on the supported formats. Compression is optional and defaults to gzip (.gz). Returns a download key. Asynchronous.
Download	Given a list key, prepare for download a file containing those records in the selected format. See the web download service documentation (http://pubchem.ncbi.nlm.nih.gov/pc_fetch/pc_fetch-help.html) for more detail on the supported formats and file types. Returns a download key. Asynchronous. Note that if SynchronousSingleRecord is set to true, and the ListKey contains only a single ID, then a Base64 string of data is returned synchronously in the response, instead of going through the download file.
GetAssayColumnDescription	Get the description of column (readout) in a BioAssay, which may be the outcome, score, or a TID from the given AID. Synchronous.
GetAssayColumnDescriptions	Get the description of all columns (readouts) in a BioAssay. Synchronous.
GetAssayDescription	Get the descriptive information for a BioAssay, including the number of user-specified readouts (TIDs) and whether a score readout is present. Optionally get version and SID/CID count information. If GetFullDataBlob is set to true, then a Base64 string of data is returned in the response instead, containing the full PubChem Assay description in the requested format (ASN or XML only). Synchronous.
GetDownloadUrl	Given a download key, return an FTP URL that may be used to download the requested file. Synchronous.
GetEntrezKey	Given a list key, return an Entrez history key (db, query key, and WebEnv) corresponding to that list. Synchronous.
GetEntrezUrl	Given an Entrez history key (db, query key, and WebEnv), return an HTTP URL that may be used to view the list in Entrez. Synchronous.
GetIDList	Given a list key, return the identifiers as an array of integers. Synchronous.
GetListItemsCount	Return the number of IDs in the set represented by the given list key. Synchronous.
GetOperationStatus	Given a key for any asynchronous operation, return the status of that operation. Possible return values are: Success, the operation completed normally; HitLimit, TimeLimit: the operation finished normally, but one of the limits was reached (e.g. before the entire database was searched); ServerError, InputError, DataError, Stopped: there was a problem with the input or on the server, and the job has died; Queued: the operation is waiting its turn in the public queue; Running: the operation is in progress. Synchronous.
GetStandardizedCID	Given a structure key that has been processed by Standardize, return the corresponding PubChem Compound database CID, or an empty value if the structure is not present in PubChem. Synchronous.

Name	Description
GetStandardizedStructure	Given a structure key that has been processed by Standardize, return the chemical structure in as SMILES or InChI strings. Synchronous.
GetStandardizedStructureBase64	Given a structure key that has been processed by Standardize, return the chemical structure as ASN, XML, or SDF, returned as a Base64-encoded string. Synchronous.
GetStatusMessage	Given a key for any asynchronous operation, return any system messages (error messages, job info, etc.) associated with the operation, if any. Synchronous.
IdentitySearch	Search PubChem Compound for structures identical to the one given by the structure key input, based on a user-selected level of chemical identity: connectivity only, match isotopes and/or stereo, etc. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.
IDExchange	Convert IDs from one type to another, using any one of a variety of CID matching algorithms. Output can be a list or a downloaded file; download file compression is optional and defaults to gzip (.gz). Returns a list or download key. Asynchronous.
InputAssay	Specify an assay table from a BioAssay AID. The table may be complete, concise, or include a ListKey-specified set of readouts (TIDs). By default, all tested substances are included, but can be restricted to a ListKey-specified set of SIDs or CIDs. Returns an assay key. Synchronous.
InputEntrez	Input an Entrez history key (db, query key, and WebEnv). Returns a list key. Synchronous.
InputList	Input a set of identifiers for a PubChem database, as an array of integers. Returns a list key. Synchronous.
InputListString	Input a set of identifiers for a PubChem database, as an array of strings. Returns a list key. Synchronous.
InputListText	Input a set of identifiers for a PubChem database, as a simple string of integer values separated by commas and/or whitespace. Returns a list key. Synchronous.
InputStructure	Input a chemical structure as a simple (one-line) string, either SMILES or InChI. Returns a structure key. Synchronous.
InputStructureBase64	Input a chemical structure in ASN.1 (text or binary), XML, or SDF format. The structure must be encoded as a Base64 string. Currently only single structures are supported. Returns a structure key. Synchronous.
MFSearch	Search PubChem Compound for structures of a given molecular formula, optionally allowing elements not specified to be present. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.
ScoreMatrix	Compute a matrix of scores from one or two lists of IDs (if one, the IDs will be self-scored), of the selected type and in the selected format. Compression is optional and defaults to gzip (.gz). Returns a download key. Asynchronous.

Methods

Name	Description
SimilaritySearch2D	Search PubChem Compound for structures similar to the one given by the structure key input, based on the given Tanimoto-based similarity score. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.
Standardize	Standardize the structure given by the structure key input, using the same algorithm PubChem uses to construct the Compound database. Returns a structure key. Asynchronous.
SubstructureSearch	Search PubChem Compound for structures containing the one given by the structure key input, based on a user-selected level of chemical identity: connectivity only, match isotopes and/or stereo, etc. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.
SuperstructureSearch	Search PubChem Compound for structures contained within the one given by the structure key input, based on a user-selected level of chemical identity: connectivity only, match isotopes and/or stereo, etc. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.

Method: AssayDownload

Description


Given an assay key, prepare for download a file containing an assay data table in the selected format. See the assay query section of the PUG service documentation (<http://pubchem.ncbi.nlm.nih.gov/pug/pughelp.html>) for more detail on the supported formats. Compression is optional and defaults to gzip (.gz). Returns a download key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/AssayDownload>


Input

The input of this method is the argument AssayDownload having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:AssayKey	s:string	1..1
tns:AssayFormat	tns:AssayFormatType	1..1
tns:eCompress	tns:CompressType	0..1

Output

The output of this method is the argument AssayDownloadResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:DownloadKey	s:string	1..1

Method: Download

Description


Given a list key, prepare for download a file containing those records in the selected format. See the web download service documentation (http://pubchem.ncbi.nlm.nih.gov/pc_fetch/pc_fetch-help.html) for more detail on the supported formats and file types. Returns a download key. Asynchronous. Note that if SynchronousSingleRecord is set to true, and the ListKey contains only a single ID, then a Base64 string of data is returned synchronously in the response, instead of going through the download file.

Action

<http://pubchem.ncbi.nlm.nih.gov/Download>


Input

The input of this method is the argument Download having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1
tns:eFormat	tns:FormatType	1..1
tns:eCompress	tns:CompressType	0..1
tns:Use3D	s:boolean	0..1
tns:N3DConformers	s:int	0..1
tns:SynchronousSingleRecord	s:boolean	0..1

Output

The output of this method is the argument DownloadResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:DownloadKey	s:string	0..1
tns:DataBlob	tns:DataBlobType	0..1

Method: GetAssayColumnDescription

Description


Get the description of column (readout) in a BioAssay, which may be the outcome, score, or a TID from the given AID. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetAssayColumnDescription>


Input

The input of this method is the argument GetAssayColumnDescription having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:AID	s:int	1..1
tns:Heading	tns:HeadingType	1..1
tns:TID	s:int	0..1

Output

The output of this method is the argument GetAssayColumnDescriptionResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ColumnDescription	tns:ColumnDescriptionType	1..1

Method: GetAssayColumnDescriptions

Description


Get the description of all columns (readouts) in a BioAssay. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetAssayColumnDescriptions>


Input

The input of this method is the argument GetAssayColumnDescriptions having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:AID	s:int	1..1

Output

The output of this method is the argument GetAssayColumnDescriptionsResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ColumnDescription	tns:ColumnDescriptionType	1..*

Method: GetAssayDescription

Description


Get the descriptive information for a BioAssay, including the number of user-specified readouts (TIDs) and whether a score readout is present. Optionally get version and SID/CID count information. If GetFullDataBlob is set to true, then a Base64 string of data is returned in the response instead, containing the full PubChem Assay description in the requested format (ASN or XML only). Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetAssayDescription>


Input

The input of this method is the argument GetAssayDescription having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:AID	s:int	1..1
tns:GetVersion	s:boolean	0..1
tns:GetCounts	s:boolean	0..1
tns:GetFullDataBlob	s:boolean	0..1
tns:eFormat	tns:FormatType	0..1

Output

The output of this method is the argument GetAssayDescriptionResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:AssayDescription	tns:AssayDescriptionType	0..1
tns:DataBlob	tns:DataBlobType	0..1

Method: GetDownloadUrl

Description


Given a download key, return an FTP URL that may be used to download the requested file. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetDownloadUrl>


Input

The input of this method is the argument GetDownloadUrl having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:DownloadKey	s:string	1..1

Output

The output of this method is the argument GetDownloadUrlResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:url	s:string	1..1

Method: GetEntrezKey

Description

Given a list key, return an Entrez history key (db, query key, and WebEnv) corresponding to that list.
Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetEntrezKey>

Input

The input of this method is the argument GetEntrezKey having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:ListKey	s:string	1..1

Output

The output of this method is the argument GetEntrezKeyResponse having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:EntrezKey	tns:EntrezKey	1..1

Method: GetEntrezUrl

Description


Given an Entrez history key (db, query key, and WebEnv), return an HTTP URL that may be used to view the list in Entrez. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetEntrezUrl>


Input

The input of this method is the argument GetEntrezUrl having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:EntrezKey	tns:EntrezKey	1..1

Output

The output of this method is the argument GetEntrezUrlResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:url	s:string	1..1

Method: GetIDList

Description


Given a list key, return the identifiers as an array of integers. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetIDList>


Input

The input of this method is the argument GetIDList having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1
tns:Start	s:int	0..1
tns:Count	s:int	0..1

Output

The output of this method is the argument GetIDListResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:IDList	tns:ArrayOfInt	1..1

Method: GetListItemsCount

Description


Return the number of IDs in the set represented by the given list key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetListItemsCount>


Input

The input of this method is the argument GetListItemsCount having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Output

The output of this method is the argument GetListItemsCountResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:count	s:int	1..1

Method: GetOperationStatus

Description

Given a key for any asynchronous operation, return the status of that operation. Possible return values are: Success, the operation completed normally; HitLimit, TimeLimit: the operation finished normally, but one of the limits was reached (e.g. before the entire database was searched); ServerError, InputError, DataError, Stopped: there was a problem with the input or on the server, and the job has died; Queued: the operation is waiting its turn in the public queue; Running: the operation is in progress. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetOperationStatus>

Input

The input of this method is the argument GetOperationStatus of type tns:AnyKeyType having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:AnyKey	s:string	1..1

Output

The output of this method is the argument GetOperationStatusResponse having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:status	tns:StatusType	1..1

Method: GetStandardizedCID

Description


Given a structure key that has been processed by Standardize, return the corresponding PubChem Compound database CID, or an empty value if the structure is not present in PubChem. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetStandardizedCID>


Input

The input of this method is the argument GetStandardizedCID having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1

Output

The output of this method is the argument GetStandardizedCIDResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:CID	s:int	1..1

Method: GetStandardizedStructure

Description


Given a structure key that has been processed by Standardize, return the chemical structure in as SMILES or InChI strings. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetStandardizedStructure>


Input

The input of this method is the argument GetStandardizedStructure having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1
tns:format	tns:FormatType	1..1

Output

The output of this method is the argument GetStandardizedStructureResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:structure	s:string	1..1

Method: GetStandardizedStructureBase64

Description


Given a structure key that has been processed by Standardize, return the chemical structure as ASN, XML, or SDF, returned as a Base64-encoded string. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetStandardizedStructureBase64>


Input

The input of this method is the argument GetStandardizedStructureBase64 having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1
tns:format	tns:FormatType	1..1

Output

The output of this method is the argument GetStandardizedStructureBase64Response having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:structure	s:base64Binary	1..1

Method: GetStatusMessage

Description

Given a key for any asynchronous operation, return any system messages (error messages, job info, etc.) associated with the operation, if any. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/GetStatusMessage>

Input

The input of this method is the argument GetStatusMessage of type tns:AnyKeyType having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:AnyKey	s:string	1..1

Output

The output of this method is the argument GetStatusMessageResponse having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:message	s:string	1..1

Method: IdentitySearch

Description


Search PubChem Compound for structures identical to the one given by the structure key input, based on a user-selected level of chemical identity: connectivity only, match isotopes and/or stereo, etc. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/IdentitySearch>


Input

The input of this method is the argument IdentitySearch having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1
tns:idOptions	tns:IdentitySearchOptions	1..1
tns:limits	tns:LimitsType	0..1

Output

The output of this method is the argument IdentitySearchResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: IDExchange

Description


Convert IDs from one type to another, using any one of a variety of CID matching algorithms. Output can be a list or a downloaded file; download file compression is optional and defaults to gzip (.gz). Returns a list or download key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/IDExchange>


Input

The input of this method is the argument IDExchange having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:InputListKey	s:string	1..1
tns:Operation	tns:IDOperationType	1..1
tns:OutputType	tns:PCIDType	1..1
tns:OutputSourceName	s:string	0..1
tns:OutputFormat	tns:IDOutputFormatType	1..1
tns:ToWebEnv	s:string	0..1
tns:eCompress	tns:CompressType	0..1

Output

The output of this method is the argument IDExchangeResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	0..1
tns:DownloadKey	s:string	0..1

Method: InputAssay

Description


Specify an assay table from a BioAssay AID. The table may be complete, concise, or include a ListKey-specified set of readouts (TIDs). By default, all tested substances are included, but can be restricted to a ListKey-specified set of SIDs or CIDs. Returns an assay key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/InputAssay>


Input

The input of this method is the argument InputAssay having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:AID	s:int	1..1
tns:Columns	tns:AssayColumnsType	1..1
tns:ListKeyTIDs	s:string	0..1
tns:ListKeySCIDs	s:string	0..1
tns:OutcomeFilter	tns:AssayOutcomeFilterType	0..1

Output

The output of this method is the argument InputAssayResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:AssayKey	s:string	1..1

Method: InputEntrez

Description


Input an Entrez history key (db, query key, and WebEnv). Returns a list key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/InputEntrez>


Input

The input of this method is the argument InputEntrez having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:EntrezKey	tns:EntrezKey	1..1

Output

The output of this method is the argument InputEntrezResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: InputList

Description


Input a set of identifiers for a PubChem database, as an array of integers. Returns a list key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/InputList>


Input

The input of this method is the argument InputList having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ids	tns:ArrayOfInt	1..1
tns:idType	tns:PCIDType	1..1

Output

The output of this method is the argument InputListResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: InputListString

Description


Input a set of identifiers for a PubChem database, as an array of strings. Returns a list key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/InputListString>


Input

The input of this method is the argument InputListString having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:strids	tns:ArrayOfString	1..1
tns:idType	tns:PCIDType	1..1
tns:SourceName	s:string	0..1

Output

The output of this method is the argument InputListStringResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: InputListText

Description


Input a set of identifiers for a PubChem database, as a simple string of integer values separated by commas and/or whitespace. Returns a list key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/InputListText>


Input

The input of this method is the argument InputListText having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ids	s:string	1..1
tns:idType	tns:PCIDType	1..1

Output

The output of this method is the argument InputListTextResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: InputStructure

Description


Input a chemical structure as a simple (one-line) string, either SMILES or InChI. Returns a structure key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/InputStructure>


Input

The input of this method is the argument InputStructure having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:structure	s:string	1..1
tns:format	tns:FormatType	1..1

Output

The output of this method is the argument InputStructureResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1

Method: InputStructureBase64

Description

Input a chemical structure in ASN.1 (text or binary), XML, or SDF format. The structure must be encoded as a Base64 string. Currently only single structures are supported. Returns a structure key. Synchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/InputStructureBase64>

Input

The input of this method is the argument InputStructureBase64 having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:structure	s:base64Binary	1..1
tns:format	tns:FormatType	1..1

Output

The output of this method is the argument InputStructureBase64Response having the structure defined by the following table.

Element	Type	Occurs
SEQUENCE		1..1
tns:StrKey	s:string	1..1

Method: MFSearch

Description


Search PubChem Compound for structures of a given molecular formula, optionally allowing elements not specified to be present. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/MFSearch>


Input

The input of this method is the argument MFSearch having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:MF	s:string	1..1
tns:mfOptions	tns:MFSearchOptions	0..1
tns:limits	tns:LimitsType	0..1

Output

The output of this method is the argument MFSearchResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: ScoreMatrix

Description


Compute a matrix of scores from one or two lists of IDs (if one, the IDs will be self-scored), of the selected type and in the selected format. Compression is optional and defaults to gzip (.gz). Returns a download key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/ScoreMatrix>


Input

The input of this method is the argument ScoreMatrix having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1
tns:SecondaryListKey	s:string	0..1
tns:ScoreType	tns:ScoreTypeType	1..1
tns:MatrixFormat	tns:MatrixFormatType	1..1
tns:eCompress	tns:CompressType	0..1
tns:N3DConformers	s:int	0..1
tns:No3DParent	s:boolean	0..1

Output

The output of this method is the argument ScoreMatrixResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:DownloadKey	s:string	1..1

Method: SimilaritySearch2D

Description


Search PubChem Compound for structures similar to the one given by the structure key input, based on the given Tanimoto-based similarity score. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/SimilaritySearch2D>


Input

The input of this method is the argument SimilaritySearch2D having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1
tns:simOptions	tns:SimilaritySearchOptions	1..1
tns:limits	tns:LimitsType	0..1

Output

The output of this method is the argument SimilaritySearch2DResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: Standardize

Description


Standardize the structure given by the structure key input, using the same algorithm PubChem uses to construct the Compound database. Returns a structure key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/Standardize>


Input

The input of this method is the argument Standardize having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1

Output

The output of this method is the argument StandardizeResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1

Method: SubstructureSearch

Description


Search PubChem Compound for structures containing the one given by the structure key input, based on a user-selected level of chemical identity: connectivity only, match isotopes and/or stereo, etc. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/SubstructureSearch>


Input

The input of this method is the argument SubstructureSearch having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1
tns:ssOptions	tns:StructureSearchOptions	0..1
tns:limits	tns:LimitsType	0..1

Output

The output of this method is the argument SubstructureSearchResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Method: SuperstructureSearch

Description


Search PubChem Compound for structures contained within the one given by the structure key input, based on a user-selected level of chemical identity: connectivity only, match isotopes and/or stereo, etc. The search may be limited by elapsed time or number of records found, or restricted to search only within a previous result set (given by a list key). Returns a list key. Asynchronous.

Action

<http://pubchem.ncbi.nlm.nih.gov/SuperstructureSearch>


Input

The input of this method is the argument SuperstructureSearch having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:StrKey	s:string	1..1
tns:ssOptions	tns:StructureSearchOptions	0..1
tns:limits	tns:LimitsType	0..1

Output

The output of this method is the argument SuperstructureSearchResponse having the structure defined by the following table.

Element	Type	Occurs
 SEQUENCE		1..1
tns:ListKey	s:string	1..1

Complex Types: PUG SOAP

Complex Types

Name
tns:AnyKeyType
tns:ArrayOfInt
tns:ArrayOfString
tns:ArrayOfTargets
tns:AssayDescriptionType
tns:AssayTargetType
tns:ColumnDescriptionType
tns:DataBlobType
tns:EntrezKey
tns:IdentitySearchOptions
tns:LimitsType
tns:MFSearchOptions
tns:SimilaritySearchOptions
tns:StructureSearchOptions
tns:TestedConcentrationType


Complex Type: tns:AnyKeyType

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:AnyKey	s:string	1..1


Complex Type: tns:ArrayOfInt

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:int	s:int	1..*


Complex Type: tns:ArrayOfString

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:string	s:string	1..*


Complex Type: tns:ArrayOfTargets

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:Target	tns:AssayTargetType	1..*


Complex Type: tns:AssayDescriptionType

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:Name	s:string	0..1
tns:Description	tns:ArrayOfString	0..1
tns:Protocol	tns:ArrayOfString	0..1
tns:Comment	tns:ArrayOfString	0..1
tns:NumberOfTIDs	s:int	1..1
tns:HasScore	s:boolean	1..1
tns:Method	s:string	0..1
tns:Targets	tns:ArrayOfTargets	0..1
tns:Version	s:int	0..1
tns:Revision	s:int	0..1
tns:LastDataChange	s:int	0..1
tns:SIDCountAll	s:int	0..1
tns:SIDCountActive	s:int	0..1
tns:SIDCountInactive	s:int	0..1
tns:SIDCountInconclusive	s:int	0..1
tns:SIDCountUnspecified	s:int	0..1
tns:SIDCountProbe	s:int	0..1
tns:CIDCountAll	s:int	0..1
tns:CIDCountActive	s:int	0..1
tns:CIDCountInactive	s:int	0..1
tns:CIDCountInconclusive	s:int	0..1
tns:CIDCountUnspecified	s:int	0..1
tns:CIDCountProbe	s:int	0..1


Complex Type: tns:AssayTargetType

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:gi	s:int	1..1
tns:Name	s:string	0..1


Complex Type: tns:ColumnDescriptionType

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:Heading	tns:HeadingType	1..1
tns:TID	s:int	0..1
tns:Name	s:string	1..1
tns:Description	tns:ArrayOfString	0..1
tns:Type	s:string	1..1
tns:Unit	s:string	0..1
tns:TestedConcentration	tns:TestedConcentrationType	0..1
tns:ActiveConcentration	s:boolean	0..1


Complex Type: tns:DataBlobType

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:Data	s:base64Binary	1..1
tns:BlobFormat	tns:BlobFormatType	0..1
tns:eCompress	tns:CompressType	0..1


Complex Type: tns:EntrezKey

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:db	s:string	1..1
tns:key	s:string	1..1
tns:webenv	s:string	1..1


Complex Type: tns:IdentitySearchOptions

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:elIdentity	tns:IdentityType	1..1
tns:ToWebEnv	s:string	0..1


Complex Type: tns:LimitsType

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:seconds	s:int	0..1
tns:maxRecords	s:int	0..1
tns:ListKey	s:string	0..1


Complex Type: tns:MFSearchOptions

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:AllowOtherElements	s:boolean	1..1
tns:ToWebEnv	s:string	0..1


Complex Type: tns:SimilaritySearchOptions

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:threshold	s:int	1..1
tns:ToWebEnv	s:string	0..1


Complex Type: tns:StructureSearchOptions

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:MatchIsotopes	s:boolean	0..1
tns:MatchCharges	s:boolean	0..1
tns:MatchTautomers	s:boolean	0..1
tns:RingsNotEmbedded	s:boolean	0..1
tns:SingeDoubleBondsMatch	s:boolean	0..1
tns:ChainsMatchRings	s:boolean	0..1
tns:StripHydrogen	s:boolean	0..1
tns:eStereo	tns:StereoType	0..1
tns:ToWebEnv	s:string	0..1


Complex Type: tns:TestedConcentrationType

Derived By

Restricting s:anyType

Content Model

Contains elements as defined in the following table.

Component	Type	Occurs
 SEQUENCE		1..1
tns:Concentration	s:double	1..1
tns:Unit	s:string	1..1

Simple Types: PUG SOAP

Simple Types

Name
tns:AssayColumnsType
tns:AssayFormatType
tns:AssayOutcomeFilterType
tns:BlobFormatType
tns:CompressType
tns:FormatType
tns:HeadingType
tns:IdentityType
tns:IDOperationType
tns:IDOutputFormatType
tns:MatrixFormatType
tns:PCIDType
tns:ScoreTypeType
tns:StatusType
tns:StereoType

Simple Type: tns:AssayColumnsType

Derived By

Restricting s:string

Enumeration

Value
eAssayColumns_Complete
eAssayColumns_Concise
eAssayColumns_TIDs

Simple Type: tns:AssayFormatType

Derived By

Restricting s:string

Enumeration

Value
eAssayFormat_XML
eAssayFormat_ASN_Text
eAssayFormat_ASN_Binary
eAssayFormat_CSV

Simple Type: tns:AssayOutcomeFilterType

Derived By

Restricting s:string

Enumeration

Value
eAssayOutcome_All
eAssayOutcome_Inactive
eAssayOutcome_Active
eAssayOutcome_Inconclusive
eAssayOutcome_Unspecified

Simple Type: tns:BlobFormatType

Derived By

Restricting s:string

Enumeration

Value
eBlobFormat_Unspecified
eBlobFormat_ASNB
eBlobFormat_ASNT
eBlobFormat_XML
eBlobFormat_SDF
eBlobFormat_CSV
eBlobFormat_Text
eBlobFormat_HTML
eBlobFormat_PNG
eBlobFormat_Other

Simple Type: tns:CompressType

Derived By

Restricting s:string

Enumeration

Value
eCompress_None
eCompress_GZip
eCompress_BZip2

Simple Type: tns:FormatType

Derived By

Restricting s:string

Enumeration

Value
eFormat_ASNB
eFormat_ASNT
eFormat_XML
eFormat_SDF
eFormat_SMILES
eFormat_InChI
eFormat_Image
eFormat_Thumbnail

Simple Type: tns:HeadingType

Derived By

Restricting s:string

Enumeration

Value
TID
outcome
score

Simple Type: tns:IdentityType

Derived By

Restricting s:string

Enumeration

Value
elidentity_SameConnectivity
elidentity_AnyTautomer
elidentity_SameStereo
elidentity_SameIsotope
elidentity_SameStereoIsotope
elidentity_SameNonconflictStereo
elidentity_SameIsotopeNonconflictStereo

Simple Type: tns:IDOperationType

Derived By

Restricting s:string

Enumeration

Value
eIDOperation_Same
eIDOperation_SameStereo
eIDOperation_SameIsotope
eIDOperation_SameConnectivity
eIDOperation_SameParent
eIDOperation_SameParentStereo
eIDOperation_SameParentIsotope
eIDOperation_SameParentConnectivity
eIDOperation_Similar2D
eIDOperation_Similar3D

Simple Type: tns:IDOutputFormatType

Derived By

Restricting s:string

Enumeration

Value
eIDOutputFormat_Entrez
eIDOutputFormat_FileList
eIDOutputFormat_FilePair

Simple Type: tns:MatrixFormatType

Derived By

Restricting s:string

Enumeration

Value
eMatrixFormat_CSV
eMatrixFormat_IdIdScore

Simple Type: tns:PCIDType

Derived By

Restricting s:string

Enumeration

Value
eID_CID
eID_SID
eID_AID
eID_TID
eID_ConformerID
eID_SourceID
eID_InChI
eID_InChIKey

Simple Type: tns:ScoreTypeType

Derived By

Restricting s:string

Enumeration

Value
eScoreType_Sim2DSubs
eScoreType_ShapeOpt3D
eScoreType_FeatureOpt3D

Simple Type: tns:StatusType

Derived By

Restricting s:string

Enumeration

Value
eStatus_Unknown
eStatus_Success
eStatus_ServerError
eStatus_HitLimit
eStatus_TimeLimit
eStatus_InputError
eStatus_DataError
eStatus_Stopped
eStatus_Running
eStatus_Queued

Simple Type: tns:StereoType

Derived By

Restricting s:string

Enumeration

Value
eStereo_Ignore
eStereo_Exact
eStereo_Relative
eStereo_NonConflicting

Index

A

AnyKeyType	37
ArrayOfInt	38
ArrayOfString	39
ArrayOfTargets	40
AssayColumnsType	53
AssayDescriptionType	41
AssayDownload	6
AssayFormatType	54
AssayOutcomeFilterType	55
AssayTargetType	42

B

BlobFormatType	56
----------------	----

C

ColumnDescriptionType	43
Complex Types	36
CompressType	57

D

DataBlobType	44
Download	7

E

EntrezKey	45
-----------	----

F

FormatType	58
------------	----

G

GetAssayColumnDescription	8
---------------------------	---

GetAssayColumnDescriptions	9
GetAssayDescription	10
GetDownloadUrl	11
GetEntrezKey	12
GetEntrezUrl	13
GetIDList	14
GetListItemsCount	15
GetOperationStatus	16
GetStandardizedCID	17
GetStandardizedStructure	18
GetStandardizedStructureBase64	19
GetStatusMessage	20

H

HeadingType	59
-------------	----

I

IdentitySearch	21
IdentitySearchOptions	46
IdentityType	60
IDExchange	22
IDOperationType	61
IDOutputFormatType	62
InputAssay	23
InputEntrez	24
InputList	25
InputListString	26
InputListText	27
InputStructure	28
InputStructureBase64	29

L

ScoreTypeType	65
SimilaritySearch2D	32
SimilaritySearchOptions	49
Simple Types	52
Standardize	33
StatusType	66
StereoType	67
StructureSearchOptions	50
SubstructureSearch	34
SuperstructureSearch	35
T	
TestedConcentrationType	51